Benzamide, 4-amino-N-[2-(diethylamino)ethyl]-

Other names:	Benzamide, 4-amino-N-[2-(diethylamino)ethyl]-
	Benzamide, p-amino-N-[2-(diethylamino)ethyl]-
	p-Amino-N-(2-diethylaminoethyl)benzamide
	p-Aminobenzoic diethylaminoethylamide
	Novocainamid
	Novocainamide
	Novocaine amide
	Novocamid
	Procaine amide
	Procamide
	Biocoryl
	Procapan (free base)
	Pronestyl
	2-Diethylaminoethylamid kyseliny p-aminobenzoove
	4-Amino-N-(diethylaminoethyl)benzamide
	NSC 27461
Inchi:	InChI=1S/C13H21N3O/c1-3-16(4-2)10-9-15-13(17)11-5-7-12(14)8-6-11/h5-8H,3-4,9-10,1
InchiKey:	REQCZEXYDRLIBE-UHFFFAOYSA-N
Formula:	C13H21N3O
SMILES:	CCN(CC)CCNC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	235.33

Physical Properties

Property code	Value	Unit	Source
hfus	37.99	kJ/mol	Joback Method
ie	7.90	eV	Cheméo Relay (1.0)
log10ws	-1.70		Cheméo Relay (1.0)
logp	1.340		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
rinpol	2193.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2248.00		NIST Webbook
rinpol	2245.00		NIST Webbook
rinpol	2193.00		NIST Webbook

tb	630.70	K	Cheméo Relay (1.0)
tf	349.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.45	J/mol×K	717.51	Joback Method
cpg	588.30	J/mol×K	752.57	Joback Method
cpg	602.18	J/mol×K	787.63	Joback Method
cpg	615.14	J/mol×K	822.69	Joback Method
cpg	627.23	J/mol×K	857.75	Joback Method
cpg	638.49	J/mol×K	892.80	Joback Method
cpg	648.98	J/mol×K	927.86	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51069&Units=SI

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point